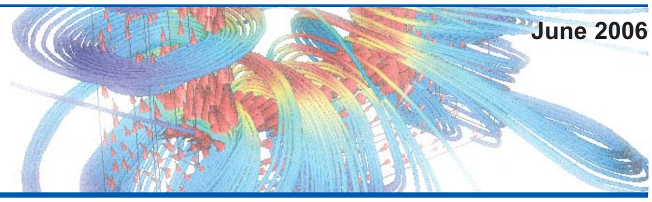
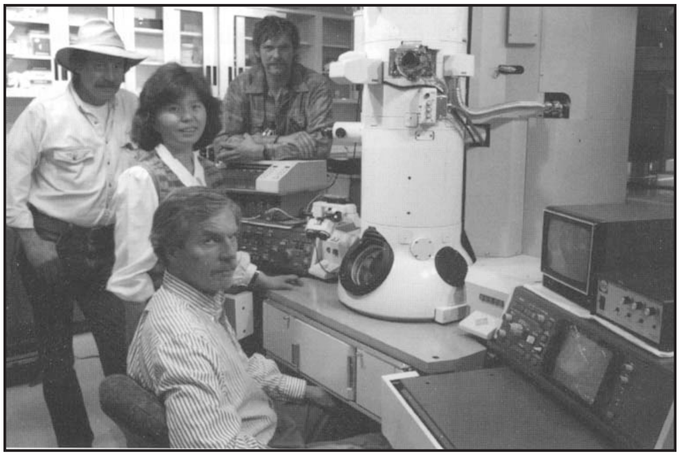
MPA material matters



June 2006

Newsletter of the Materials Physics and Applications Division



We must always change, renew, rejuvenate ourselves; otherwise we harden.

Goethe

Transition has meant change, but even with the creation of the new Materials Science and Technology and the Materials Physics and Applications Divisions, familiar faces remain.

Pictured clockwise from upper left: Jim Smith, Harriet Kung, Terry Mitchell and Kurt Sickafus; Manuel Jaramillo, John Balog, David Sandoval, and Richard Less; Susie Duran, Ross Lemons and Laurie Lauer; Tom Bell, Ray Dixon, Tim Darling, Bill Visscher, Albert Migliori; Paul Arendt, Xin Di Wu and Steve Foltyn; Dave Korzekwa, John Bingert and Ralph Trujillo; Bob Carpenter and Carl Trujillo.

From John's desk...

Materials Physics and Applications: Three weeks and counting...

As I write the first Materials Physics and Applications "From the Desk," our organization is approaching its three-week anniversary. My perception—I'd welcome hearing your perspectives—is that we're off to a good start with no major disasters (yet). From my calls to your group offices, it's clear that our new organization names are a mouthful (and I've caught myself several times answering my phone "MST Division"). We're working on improved names/acronyms and you should see institutional guidance on this soon. We've also had a few hiccups with authorities and foreign travel approvals. By and large, however, work is getting done and I very much appreciate the sense of optimism that I perceive when I talk to all of you in meetings and in walkarounds.

Planning for next fiscal year and beyond is well underway. With your group leaders, we have developed a short-term hiring plan to address actions that got "stuck" in the transition and to fill other key strategic needs. Associate Director for Experimental Physical Sciences Susan Seestrom has approved this plan and we're working to implement it. I spent a Sunday and Monday earlier this month in a planning retreat for the weapons physics part of the NNSA budget; I'm confident that a greater focus on mission capabilities and strategic capabilities will emerge that should benefit a number of efforts within MPA. Finally, the first of the new Director's Science and Technology Portfolio Reviews occurred this week. MPA has the largest portfolio of any division within Terry Wallace's program offices and we were mentioned early and often relative to our recent successes.

Another sign of summer is the significant number of students that are arriving at the Laboratory. I hope to schedule in the very near future an "MPA Students All-Hands" meeting so that I can have a chance to visit with and meet our Division's students. My own time at the Laboratory began as a summer student, so I appreciate firsthand both how rewarding an experience it can be, but also how confusing life at LANL is for newcomers (even without a contract transition added to the mix). Please make a specific effort to welcome the students in your organization to MPA and share with them your excitement for the future.

Finally, I would like to end on a safety note. Given all the changes that are afoot around the Laboratory, the influx of students and other visitors, and the various vacation plans that we all have, it is quite easy to become distracted and lose focus on the task at hand. Please deliberately resist this temptation by focusing on the five steps of integrated work management in all that you do. We should have no higher priority than that each of you goes home at least as safe and healthy each night as you were when you arrived that morning.

I look forward to meeting more of you in the weeks and months ahead and to the success of our new organization.

— John Sarrao, MPA Division Leader

p.s. The MPA Division Office is located in the Materials Science Laboratory (where MST-DO used to be) and we've kept the MST phone number: 5-1131

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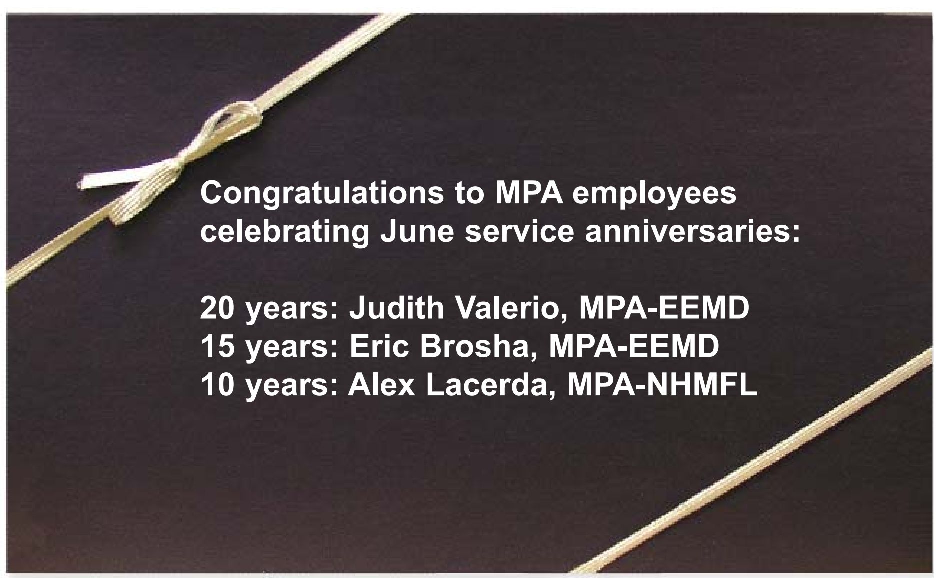
Celebrating service

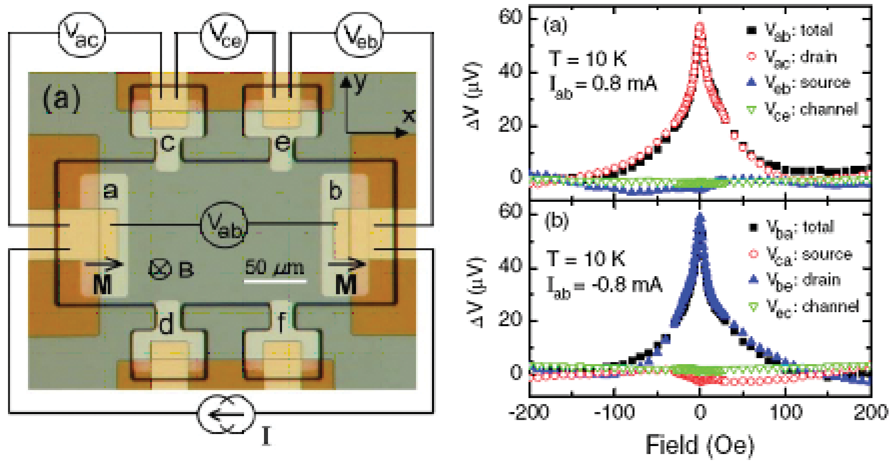


Research reveals new method of detecting spin-polarized electron accumulation

New research by scientists at LANL's National High Magnetic Field Laboratory in collaboration with scientists at the University of Minnesota shows that it is possible to electrically detect the accumulation of spin-polarized electrons that occurs when electrical current flows from a semiconductor (gallium arsenide) into a ferromagnetic metal (iron).

Traditionally, polarization-sensitive optical techniques are used to measure the spin polarization of electrons in semiconductors. However, any practically useful "semiconductor spintronic" device of the future must employ an all-electrical scheme to measure electron spin polarization.

In devices incorporating Fe/GaAs Schottky tunnel barriers, spin accumulation leads to an additional voltage drop across the barrier that is suppressed by a small transverse magnetic field, which depolarizes the spins in the semiconductor. The dependence of the electrical accumulation signal on magnetic field, bias current, and temperature is in good agreement with the predictions of a drift-diffusion model for spin-polarized transport.



(left) Photomicrograph of the Fe/GaAs spin transport device. The side contacts are used for the voltage measurements indicated by the labels.
(right) (a) Voltage vs. in-plane magnetic field (By) for an electron current flowing from contact b (the source) to contact a (the drain). The source-drain voltage Vab=0.5 V. (b) Measurements with the current reversed (electrons now flowing from flowing from a to b). The extra voltage peak at zero magnetic field appears only for measurements that include the drain contact, and is due to an accumulated spin polarization at the drain.

This work, "Electrical Detection of Spin Accumulation at a Ferromagnet-Semiconductor Interface", by Xiaohua Lou, Christoph Adelmann, Chris Palmstrom and Paul Crowell, University of Minnesota, working in collaboration with Madalina Furis and Scott Crooker, MPA-NHMFL, will be published in an upcoming issue of *Physical Review Letters*.

Los Alamos and MetOx collaborate to accelerate availability of commercial HTS wire

Los Alamos National Laboratory and Metal Oxide Technologies of Houston have signed a cooperative research and development agreement (CRADA) in an effort to significantly accelerate the availability of high current, long-length, high-temperature superconducting (HTS) wire for the transmission of enormous amounts of electricity without loss or heat.

> **"The Laboratory is fully committed to assist the Department of Energy in reaching its objective of having a healthy, multi-company, high-temperature superconductivity industry in place by 2010."**
>
> *Dean Peterson*
> *MPA-STC center leader*

LANL will provide the benefit of its 20 years of superconductivity research and development to the CRADA with MetOx with the objective to fabricate wire with the ability to transmit unprecedented amounts of electricity through wires created by a MetOx-modified metal organic chemical vapor deposition process originally developed at the University of Houston. This process currently produces HTS wire capable of transmitting more than 150 times more electric power than conventional copper wire.

The Laboratory will supply ion-beam assisted deposition template buffered metallic substrate for superconductor deposition, characterize the properties and microstructure of the enhanced MetOx wire and provide feedback to MetOx regarding its wire development effort. MPA's Superconductivity Technology Center (MPA-STC) will be the location for the fabrication and characterization effort.

MetOx expects to start producing long lengths of second generation HTS wire this year in Houston. The development of ion-beam assisted deposition textured template technology at Los Alamos helped further the use of high-temperature superconductors, such as yttrium-barium-copper-oxide.

"The Laboratory is fully committed to assist the Department of Energy in reaching its objective of having a healthy, multi-company, high-temperature superconductivity industry in place by 2010. This CRADA with MetOx will assist the DOE in achieving this goal," said Dean Peterson, STC center leader.

Superconducting technology will enable the more efficient generation of electricity. Ten percent of the electricity generated in the United States each year (300 million kilowatt hours) is lost due to resistance in copper and aluminum wires. Based on these numbers, HTS technology will improve electric transmission efficiency and save more than $1 billion per year in electrical losses. Other benefits will be more compact transmission cables and lighter, smaller motors and generators. MetOx has applied for 23 U.S. and foreign patents. Los Alamos' effort is funded by DOE's Office of Electricity Delivery and Energy Reliability, Superconductivity Program for Electric Systems.

Research on shape memory effect leaves lasting impression

A National High Magnetic Field Laboratory (MPA-NHMFL)-led paper on shape memory effect is leaving a lasting impression on the world of condensed matter physics

"Fermi surface as a driver for the shape-memory effect in AuZn" has been chosen by the *Journal of Physics:Condensed Matter* as one of the top papers of 2005. The papers and review articles chosen for the 2005 showcase are considered to be the very best contributions of the last year.

"It makes all the long nights in the lab worthwhile when the result provokes so much interest," said Ross McDonald, MPA-NHMFL, the paper's lead author.

The paper greatly contributes to the advancement of materials science. As summarized in the showcase summary, "the data and calculations provide direct evidence about the role of the band-electron system and its Fermi surface in the shape memory effect, showing that band-structure/property relations are an important consideration for the design of future shape memory alloys." Richard Palmer, publisher of the journal, said the top papers received the highest praise from the board referees and were the most highly downloaded articles throughout 2005.

Alex Lacerda, director of the Pulsed Field Facility, said McDonald and his LANL colleagues are very deserving of the recognition. "Having a staff with such rich research of its own is one reason why our user's program remains among the best in the world," Lacerda said.

McDonald's co-authors include John Singleton, Paul Goddard, Fivos Drymiotis, Neil Harrison, Albert Migliori, MPA-NHMFL; James L. Smith, Jason C. Lashley, MST-6; H. Harima and M.T. Suzuki Osaka University, Kobe University; A. Saxena, T-CMSP; and Tim Darling, MPA-CMTP.

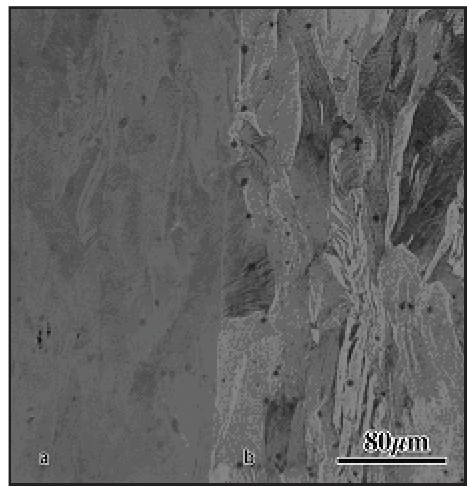
New technique offers more environmentally acceptable metallographic preparation techniques for uranium

Existing metallographic preparation techniques for uranium are limited to elucidating specific microstructural characteristics, and some of the techniques are regarded as environmentally unacceptable.

In "Metallographic preparation techniques for uranium," to be published in an upcoming issue of *Journal of Nuclear Materials*, Ann Kelly, MST-6, describes a newly developed technique which is not only more environmentally acceptable, but reveals most microstructural features simultaneously.

Example microstructures of the various preparation stages are shown at right to highlight the new technique.

At right, a differential interference contrast micrograph illustrating the differences in microstructural clarity of a cold-rolled uranium specimen for (a) mechanical polished surface (through 1 μm diamond) and (b) subsequently electropolished surface, after allowing the specimen to oxidize in air.



Scientists extend parallel-replica dynamics to driven systems

Though a powerful tool for probing atomic-scale materials properties, molecular dynamics (MD) simulations can typically only access timescales of nanoseconds to microseconds, while many relevant physical phenomena occur on much longer timescales.

Accelerated dynamics methods, developed at Los Alamos, overcome this limitation of MD.

In this work, conducted by scientists in LANL's Materials Science and Technology and Theoretical Divisions as well as at Clemson University, researchers show that parallel-replica dynamics, one of the accelerated dynamics methods, can be extended to driven systems, e.g., systems with time-dependent boundary conditions.

They show that as long as the system is driven slowly enough so that the rates to escape a state do not depend on the time history of the drive, the state-to-state dynamics are correct.

Researchers are able to perform simulations in weeks that would take the better part of a year to perform on a single processor.

The scientists demonstrate the algorithm by stretching a carbon nanotube with a preexisting vacancy, noting a significant dependence of the nature of nanotube yield on the strain rate.

In particular, they are able to achieve strain rates slow enough such that the time scale for vacancy diffusion is faster than that for mechanical yield at a temperature of 2000 K.

Thus they observe vacancy-induced morphological changes in the nanotube structure, providing some insight into previously unexplained experimental features. This method has also been applied to the problem of grain boundary sliding, work which is being prepared for publication.

"Parallel-Replica Dynamics for Driven Systems: Derivation and Application to Strained Nanotubes," by Blas Uberuaga, MST-8, Steven Stuart, Clemson University, and Arthur Voter, T-TCMP, has been submitted to *Physical Review B*.

Work at LANL was supported by the United States Department of Energy, Office of Basic Energy Sciences and through a cooperative research and development agreement with Motorola.

Work at Clemson was supported by the Department of Energy and the National Science Foundation.

LANL begins new collaboration on hydrogen and fuel cell research

On May 16 Los Alamos National Laboratory announced the start of a collaboration on the development of fuel cells and hydrogen technologies between Los Alamos, Japan's New Energy and Industrial Technology Development Organization (NEDO) and National Institute of Advanced Industrial Science and Technology (AIST). Formalized by a memorandum of understanding, the partnership anticipates collaborations between the Los Alamos Institute for Hydrogen and Fuel Cell Research, NEDO's Fuel Cell and Hydrogen Technology Department and AIST's Polymer Electrolyte Fuel Cell Cutting-edge Research Center covering the important technical aspects of hydrogen-powered vehicles.

The Institute for Hydrogen and Fuel Cell Research was formed in 2004 as a partnership between the Lab's Chemistry and Materials Science and Technology divisions. The institute was created to coordinate hydrogen and fuel cell research projects across the Laboratory, to improve access to Los Alamos' unique fuel cell capabilities and facilities, and to enhance the Laboratory's ability to attract high quality entry level and senior staff in the field of hydrogen energy research.

Joy ride!

Juanita Armijo, MPA-CMTP, takes a spin on the Freedom Cart, a fuel cell-powered scooter built by members of MPA-EEMD. She was taking part in a tour of the group offered to the office administrators by MPA-EEMD Group Leader Ken Stroh, pictured at right.

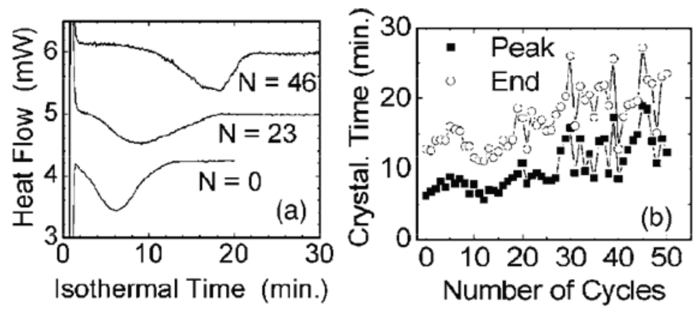
Recorded low critical cooling rate for forming bulk metallic glasses

Metallic glasses contain no crystal defects such as dislocations and grain boundaries because they posses disordered "liquid-like" atom structures that can be formed by freezing liquid metals. Therefore, compared with crystalline counterparts, metallic glasses usually show superior mechanical properties and corrosion resistance. But not until now have metallic glasses been used for structural parts because processing them usually requires an extremely high critical cooling rate (CCR), which limits the form of metallic-glass products to either powders or thin films.

Tongde Shen, in collaboration with Ricardo Schwarz, both MST-8, has obtained the lowest CCR that is needed to form a bulk metallic glass. Shen and Schwarz have found a cyclic melting and solidification method to purify palladium-based alloy melt (Shen and Schwarz, *Applied Physics Letters*, **88**, 091903 (2006)). The thermal cyclic treatment results in repeated crystallization that decreases the number of heterogeneous nucleants. The researchers think that this process is similar to the well-known zone purification techniques widely used in the metallurgical industry in which a solidification (or crystallization) front moves and traps impurities at the end of the solidification zone.

After the purification treatment, the CCR for forming bulk metallic glass can be decreased by a factor of 10, resulting in an extremely low CCR of 0.005 K/s (18 K/hour). This rate is a factor of 13 slower than the previously reported lowest CCR for all known bulk glass forming alloys.

The achieved CCR is within the cooling rate regime where standard castings and ingots are made in normal solidification processing conditions, making the industry processing of bulk metallic glasses possible. The purification method can also be applied in iron-based alloy melt to process bulk iron-based (amorphous) alloys (Shen and Schwarz, *Applied Physics Letters* 75, **49** (1999) and *Acta Materialia* **49**, 837 (2001)), which can either lower the energy loss when applied in transformers and motors or increase the mechanical strength and corrosion resistance when used to replace conventional (crystalline) steels. The invention of amorphous iron-based alloys, which have been recently named as "amorphous steels," can potentially revolutionize the steel industry (*Washington Times,* June 24, 2004) because they have a hardness and strength more than double the best ultra-high-strength conventional steels.



(a) Differential scanning calorimetry isothermal curves measured for $Pd_{44}Ni_{10}Cu_{2}6P_{20}$ during an isothermal annealing at 420 °C after 0, 23, and 46 times cyclic heating-cooling-annealing treatments. (b) crystallization peak (■) and end (O) times extracted from (a) as a function of number of cyclic heating-cooling-annealing treatments.

The research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences.

Heads UP, MPA!

A textbook evacuation

What might be considered a textbook example of a building evacuation took place June 6 at 1 p.m. Kudos go to all those involved.

A strong burning odor in an office area of Building 32 prompted the MST Facility Operations Leader to pull the fire alarm, which began the evacuation of Buildings 32, 34, 1819 and 2002.

Occupants mustered in the correct area; evacuating the buildings without eating or drinking; a majority of sweep cards were collected allowing the fire department to focus on unswept areas; and line management was fully engaged. Weather conditions caused the evacuated personnel to properly re-muster in the Materials Science Laboratory. At the direction of incident command, MST assisted in securing the building, which was not cleared for re-entry until 3 p.m.

The cause of the burning odor is under investigation.

A final note, even if in doubt about a burning odor, using the pull station to alert occupants is the correct action.

Recycling hazardous metals

Lead metal was recently discovered in an open metal recycling bin located outside of an MST facility. Although it is permissible to recycle hazardous metals, these materials should be protected from the environment when recycling. Contact your waste management coordinator (WMC) when recycling hazardous metals such as lead, cadmium, and printed circuit boards. The WMC will supply a secondary container to protect the material from the environment. After the container is marked with its contents, it will be placed in the open recycling bin.

New parking requirements

New parking requirements have gone into effect at Los Alamos National Laboratory.

In general, LANL workers, guests, and visitors may park vehicles in designated areas at LANL or LANL-leased space. LANL reserves the right to control where vehicles may be parked, how long they may be parked, and how parking areas may be used.

LANL parking facilities include parking lots, parking structures, and other designated parking areas. Designated parking areas are paved areas with painted lines, specifically-designated gravel parking lots, or parking decks designed specifically for vehicle parking.

Parking is not allowed:

- In areas where parking or leaving a vehicle would be unsafe, regardless of any parking designation, posting, or marking.
- In areas posted or designated "no parking."
- In fire lanes or safety zones identified by markings or signs.
- Within 15 feet of a fire hydrant.
- Within 20 feet of posted security fences, except where parking spaces closer than 20 have been defined by painted lines, parking bumpers, or signs.
- In locations that represent a hazard to vehicular, emergency, pedestrian traffic, physical security, or the environment.
- On sidewalks, marked pedestrian crosswalks, or landscaped areas.
- In identified areas reserved for specially authorized vehicles, such as emergency vehicles.
- Alongside streets or roads on LANL premises, unless otherwise marked or posted.

The administrative fine for illegally parking in fire lanes, safety zones, designated accessible spaces, blocking roadways or otherwise obstructing the safe flow of vehicular or pedestrian traffic is $50. These vehicles also are subject to being towed at the owner's expense. The administrative fine for all other parking violations is $20. The fee for towing a vehicle is $100.

Violators of the parking provisions of these requirements may be subject to notices, parking tickets, fines, towing and impounding his or her vehicle, loss of access, or termination of employment at LANL.

To read the new requirements, see http://policy.lanl.gov/pods/policies.nsf/MainFrameset?ReadForm&DocNum=IMP908&FileName=imp908.pdf.

New industrial hygienist

Marc Andersch is a new industrial hygienist supporting MST and MPA.

He can be reached at 6-1491 or mandersch@lanl.gov.

Who are you going to call?

The organization charts for the new Materials and Chemistry Facility Operations Directorate can be found online at http://int.lanl.gov/orgs/srops/.

There were no facility transitions to new organizations on June 1, however, an implementation plan will be distributed once completed.

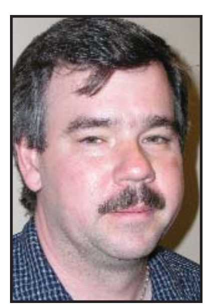
Heads UP, MPA! reports on environment, safety, and health, security, and facility-related news and information.

Who's new

As a postdoctoral researcher in MPA-CMTP, **Huidan Yu** is developing multiscale techniques to model and simulate complex flows with multiple processes. Yu holds doctorates in aerospace engineering from Texas A&M University and in physics from Peking University, China.

Postdoctoral researcher **Hao Yang** earned his doctorate from the Institute of Physics, Chinese Academy of Sciences, Beijing. He is now researching multiferroic thin films in MPA-STC.

Hershel Jude comes to Los Alamos from the University of Utah and joined MPA-CINT as a postdoctoral researcher to work on the development of photocatalytic molecular approaches to water splitting.



Before joining MPA-CINT as a technician **Jon Baldwin** worked with Ktech corporation, a subcontractor to Sandia National Laboratories. With CINT he is involved in the physical vapor deposition side of thin films synthesis.

Materials Science and Technology Division Transition Barbecue

May 31, 2006